

ENERGETICS AND CRYSTAL CHEMISTRY OF RUDDLESSEN-POPPER TYPE STRUCTURES IN HIGH  $T_c$  CERAMIC SUPERCONDUCTORS. Anurag Dwivedi and A. N. Cormack, Alfred University, Alfred, NY-14802

The formation of Ruddlesden-Popper type layers (alternating slabs of rocksalt and perovskite structures) is seen in these oxides which is similar in many respects to what is seen in the system Sr-Ti-O. However, we have observed that there are some significant differences, for example the rocksalt and perovskite blocks in new superconducting compounds are not necessarily electrically neutral, unlike in Sr-Ti-O system. This will certainly render an additional coulombic bonding energy between two different types of blocks and may well lead to significant differences in their structural chemistry.

In the higher order members of the various homologous series, additional Cu-O planes are inserted in the perovskite blocks. In order for the unit cell to be electrically neutral the net positive charge on rocksalt block (which remains constant throughout the homologous series) should be balanced by an equal negative charge on the perovskite block. It, thus, becomes necessary to create oxygen vacancies in the basic perovskite structure, when width of the perovskite slab changes on addition of extra Cu-O planes.

Results of our atomistic simulations suggest that these missing oxygen ions allow the Cu-O planes to buckle in these compounds. This is also supported by the absence of buckling in the first member of Bi-containing compounds in which there are no missing oxygen ions and the Sr-Ti-O series of compounds. We will present additional results on the phase stability of polytypoid structures in these crystal chemically complex systems. We will also focus our studies on (a) the determination of the location of  $\text{Cu}^{3+}$  in the structures of higher order members of the La-Cu-O system and (b) whether  $\text{Cu}^{3+}$  ions or oxygen vacancies are energetically more favorable charge compensating mechanism.